QUESTIONNAIRE

ASMS COMMITTEE III: COMPUTERS AND DATA PROCESSING

We encourage every ASMS member to complete this questionnaire, regardless of his present involvement in the application of computers to mass spectrometry. Please return as soon as possible.

1. Do you work for: ☐ government ☐ university ☐ industry ☐ instrument manufacturer

2. Do you: ☐ direct application of mass spectrometry ☐ acquire and/or interpret mass spectra

3. Do you use computers for processing mass spectral data? ☐ Yes ☐ No

4. If yes, is your MS-Computer system: ☐ dedicated; on-line ☐ time sharing with lab computer ☐ batch; off-line ☐ combination of above

5. If no, do you intend to use computers in mass spectrometry sometime in the future? ☐ Yes ☐ No

6. Do you feel that the goals of Committee III; The Collection and Dissemination of Mass Spectra and Software; are of value to the members of ASMS? ☐ Yes ☐ No

7. If No, what other areas of interest do you think Committee III should pursue?

_____

8. Have you ever contributed mass spectra to any spectra collection efforts? ☐ Yes ☐ No

9. If yes, estimate the amount of time per spectrum required. _____

10. Indicate as many statements below as necessary to describe your attitude toward donating mass spectra.

- ☐ I do not have any spectra to contribute
- ☐ I have too few spectra to contribute
- ☐ I have too many spectra to contribute
- ☐ I do not know the proper form to prepare spectra for submission
- ☐ My spectra are not of sufficient quality to contribute
- ☐ Preparing spectra for contribution is too much trouble
- ☐ My organization considers spectra to be proprietary
- ☐ I do not like the idea of freely given spectra appearing in commercial collections from which others may derive income
- ☐ I have no interest in this effort
- ☐ Other_____

11. Do you presently have spectra which you could contribute? ☐ Yes ☐ No

12. Have you ever given any programs to anyone? ☐ Yes ☐ No

13. If yes, were you bothered by the person in receipt of the program? ☐ Yes ☐ No

14. Have you ever received a program from anyone? ☐ Yes ☐ No

15. If yes, was the exchange of any benefit? ☐ Yes ☐ Doubtful ☐ No

16. Do you presently have programs which you could contribute? ☐ Yes ☐ No

Please express your attitude toward workshop/discussion groups in the following areas:

	Interested	No Opinion	Not Interested
A) DATA ACQUISITION converting analog data to computer-readable form	☐	☐	☐
B) DATA REDUCTION converting computer-readable data to mass spectra	☐	☐	☐
C) DATA ANALYSIS massaging mass spectral data to aid in analysis and interpretation	☐	☐	☐
D) DATA SEARCH searching reference file of mass spectra by computer	☐	☐	☐
E) HEURISTICS computer-aided interpretation of mass spectral fragmentation patterns	☐	☐	☐

Please suggest any other topics you feel appropriate for a workshop/dicussion group._____

The following items may be of interest to members of the society. If you wish to receive more detailed information on any of these items, please check the appropriate box and provide you mailing address.

NAME _____

ADDRESS _____

_____

_____

PHONE ( ) _____

☐ Results of Committee III 1973-74 survey of MS-Computer systems used by ASMS members

☐ DENDRAL programs for MS and more general applications to chemistry will be available to qualified users sometime later this year via a nationwide communications network. Policy decisions as to availability are not yet firm; however, further details will be provided to members as they are announced.

PROGRAMS

ISOTOPE DISTRIBUTION CALCULATION PROGRAM - Vander Velde

Fortran on CDC6600

Computes parent mass number vs base peak, relative intensity for molecular or atomic species entered

☐ Card deck
☐ Listing and documentation

PROGRAM FOR GAS OIL AROMATICS METHOD - Robinson and Cook

Fortran on IBM 360

Computes type analysis for 18 aromatic hydrocarbons and 3 aromatic thiophenes from mass spectra of petroleum fractions boiling within the range of 200-540°C (400-1000°F)

☐ Card deck
☐ Listing and documentation

PROGRAM FOR COMPUTING MONOISOTOPIC MASS SPECTRA AND FORMULAS - Rozett
Fortran on
Computes a least-squares-fit monoisotopic mass spectrum from polyisotopic measurements for any elements and any isotopic abundances

☐ Card deck
☐ Listing and documentation

HIGH RESOLUTION SOFTWARE PACKAGE FOR PDPI2, 8 K CORE - Crittenden

☐ Documentation only available at this time

HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP-HELP

If you are willing to contribute your time and energy to the work of Committee III please so indicate

I will Help: NAME_____

ADDRESS_____

_____

_____

PHONE ( ) _____

I can assist in the following manner: _____

THANKS-THANKS-THANKS-THANKS-THANKS-THANKS-THANKS-THANKS-THANKS-THANKS-THANKS

Please fold page so that address shows and send by return mail. Thank you.